=>

Uploading C:\Program Files\Stnexp\Queries\10662781.str

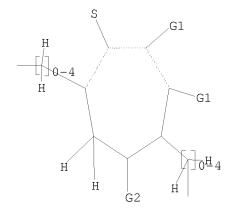
L1STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1

STR



G1 H,S

G2 H, O

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

118 ANSWERS

FULL SEARCH INITIATED 11:32:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 292237 TO ITERATE

100.0% PROCESSED 292237 ITERATIONS SEARCH TIME: 00.00.01

L2

118 SEA SSS FUL L1

L3

43 L2

 \Rightarrow s 13 and py<2002 21939595 PY<2002

L4 37 L3 AND PY<2002

=> d 1-37 ibib abs hitstr

L4 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:490629 CAPLUS

DOCUMENT NUMBER: 135:257352

TITLE: Synthesis of sulfur-containing bis-terpenoids based on

monoterpene oxides

AUTHOR(S): Startseva, V. A.; Nikitina, L. E.; Artemova, N. P.;

Dieva, S. A.; Plemenkov, V. V.

CORPORATE SOURCE: S. V. Kurashov Kazan' State Medical University,

Kazan', 420012, Russia

SOURCE: Chemistry of Natural Compounds (Translation of Khimiya

Prirodnykh Soedinenii) (2001), Volume Date

2000, 36(6), 587-589

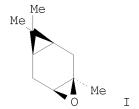
CODEN: CHNCA8; ISSN: 0009-3130

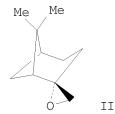
PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:257352

GΙ





AB Ethanedithiol and di(mercaptoethyl)sulfide react regio- and stereoselectively with (+)-3-carene- β -oxide (I) and β -pinene- α -oxide (II) in the presence of sodium ethoxide to give the corresponding bis- and trissulfides with two terpene fragments.

IT 361358-15-8P 361358-18-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of sulfur-containing bis-terpenoids based on monoterpene oxides)

RN 361358-15-8 CAPLUS

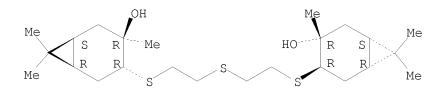
CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-[1,2-ethanediylbis(thio)]bis[3,7,7-trimethyl-, (1S,1'S,3R,3'R,4R,4'R,6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 361358-18-1 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-[thiobis(2,1-ethanediylthio)]bis[3,7,7-trimethyl-, (1S,1'S,3R,3'R,4R,4'R,6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:420854 CAPLUS

DOCUMENT NUMBER: 136:216889

TITLE: Synthesis of 4α -alkylthiocarane- 3β -thiols

AUTHOR(S): Fedyunina, I. V.; Nikitina, L. E.; Plemenkov, V. V.

CORPORATE SOURCE: S. V. Kurashov Kazan' State Med. Inst., Russia

SOURCE: Khimiya Prirodnykh Soedinenii (1992), (5),

497-499

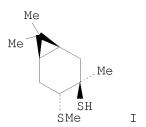
CODEN: KPSUAR; ISSN: 0023-1150

PUBLISHER: Izdatel'stvo Fan

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 136:216889

GΙ



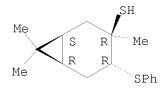
- AB Addition reactions of thiols to $\beta-3$,4-epithiocarane under conditions of base catalysis have been studied. The reaction takes place regio- and stereo-specifically with the formation of 4α -alkylthiocarane- 3β -thiols, e.g. I.
- IT 170509-59-8P 170716-52-6P 170716-54-8P 170897-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of 4α -alkylthiocarane- 3β -thiols)

RN 170509-59-8 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-(phenylthio)-, (1S,3R,4R,6R)- (CA INDEX NAME)

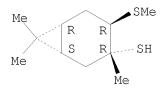
Absolute stereochemistry.



RN 170716-52-6 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-(methylthio)-, (1S,3R,4R,6R)- (CA INDEX NAME)

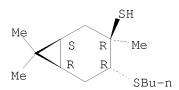
Absolute stereochemistry. Rotation (-).



RN 170716-54-8 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 4-(butylthio)-3,7,7-trimethyl-, (1S,3R,4R,6R)- (CA INDEX NAME)

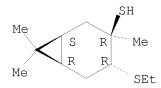
Absolute stereochemistry. Rotation (-).



RN 170897-50-4 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 4-(ethylthio)-3,7,7-trimethyl-, (1S,3R,4R,6R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:361751 CAPLUS

DOCUMENT NUMBER: 135:152572

TITLE: Strained cyclopropenes. Synthesis and reactions of

3-isopropenyl-6-methylbicyclo[4.1.0]hept-1(7)-ene in

situ

AUTHOR(S): Startseva, V. A.; Nikitina, L. E.; Plemenkov, V. V.

CORPORATE SOURCE: Kurashov Kazan State Medical University, Kazan, Russia

Russian Journal of General Chemistry (Translation of

Zhurnal Obshchei Khimii) (2000), 70(11),

1760-1762

CODEN: RJGCEK; ISSN: 1070-3632

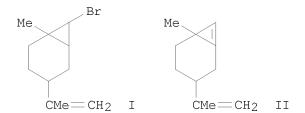
PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:152572

GΙ

SOURCE:



7-Bromo-4-isopropenyl-1-methylbicyclo[4.1.0]heptane (I), generated by electrochem. reduction of the corresponding dibromocyclopropane, reacted with strong bases to give short-lived 3-isopropenyl-6-methylbicyclo[4.1.0]hept-1(7)-ene (II), whose formation was proved by Diels-Alder reactions with isoprene and alloocimene in situ. The reaction of I with 2-mercaptoethanol in the presence of potassium tert-butoxide demonstrated the possibility of formal replacement of the bromine atom in the substrate by a sulfide moiety.

IT 352311-56-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (formation and reactions of 3-isopropenyl-6-methylbicyclo[4.1.0]hept-1(7)-ene in situ)

RN 352311-56-9 CAPLUS

CN Ethanol, 2-[[(1R,6S,7R)-1-methyl-4-(1-methylethenyl)bicyclo[4.1.0]hept-7-yl]thio]-, rel- (CA INDEX NAME)

Relative stereochemistry.

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{R} \\ & \\ \text{S} \\ & \\ \text{CH}_2 \\ \end{array}$$

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:267194 CAPLUS

DOCUMENT NUMBER: 135:31482

TITLE: Cyanide and thiocyanate-based biosynthesis in tropical

marine sponges

AUTHOR(S): Simpson, Jamie S.; Garson, Mary J.

CORPORATE SOURCE: Department of Chemistry, The University of Queensland,

Brisbane, 4072, Australia

SOURCE: ACGC Chemical Research Communications (2000

), 11, 38-44

CODEN: ACRCFA; ISSN: 1020-5586

PUBLISHER: Asian Coordinating Group for Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

AB The marine sponge Axinyssa n.sp. incorporates both sodium [14C] cyanide and sodium [14C] thiocyanate into 2-thiocyanatoneopupukeanane as well as into 9-isothiocyanatopupukeanane, however these two precursors were poorly incorporated into 9-isocyanopupukeanane. The specificity of incorporation into the thiocyanate carbon was confirmed by chemical degradation Stylotella aurantium incorporates sodium [14C] cyanide and sodium [14C] thiocyanate into the dichloroimine functionality of the stylotellanes A and B, as well as into the isothiocyanate. The specificity of incorporation into the dichloroimine carbon atom was confirmed by chemical degradation A 14C-labeled sample of bisisothiocyanatoadociane was incorporated into diisocyanoadociane by A. terpenensis.

IT 342580-08-9

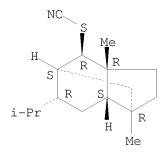
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(cyanide and thiocyanate-based biosynthesis in tropical marine sponges)

RN 342580-08-9 CAPLUS

CN Thiocyanic acid, (1R, 3aR, 4R, 5S, 6R, 7aS) -octahydro-1, 3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:85156 CAPLUS

DOCUMENT NUMBER: 134:252485

TITLE: The first total synthesis of $(\pm)-2-$

thiocyanatoneopupukeanane based on a pinacol-type

rearrangement

AUTHOR(S): Uyehara, T.; Onda, K.; Nozaki, N.; Karikomi, M.; Ueno,

M.; Sato, T.

CORPORATE SOURCE: Faculty of Engineering, Department of Applied

Chemistry, Utsunomiya University, Utsunomiya, Tochiqi,

321-8585, Japan

SOURCE: Tetrahedron Letters (2001), 42(4), 699-702

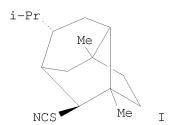
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:252485

GΙ



AB The racemic mixture of 2-thiocyanatoneopupukeanane (I), a marine sesquiterpene-thiocyanate with a tricyclo[4.3.1.03,7]decane skeleton, was prepared through a pinacol-type rearrangement of a bicyclo[2.2.2]oct-5-en-2-ol giving a bicyclo[3.2.1]oct-6-en-2-one derivative and an aldol reaction leading to the neopupukeanane framework.

IT 330840-69-2P

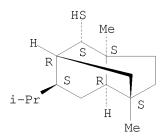
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis of (\pm) -2-thiocyanatoneopupukeanane via pinacol-type rearrangement)

RN 330840-69-2 CAPLUS

CN 1,5-Methano-1H-indene-4-thiol, octahydro-1,3a-dimethyl-6-(1-methylethyl)-, (1R,3aR,4R,5S,6R,7aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 330840-39-6P, (\pm) -2-Thiocyanatoneopupukeanane

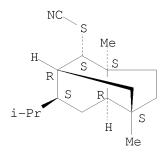
RL: SPN (Synthetic preparation); PREP (Preparation)

(total synthesis of (\pm) -2-thiocyanatoneopupukeanane via pinacol-type rearrangement)

RN 330840-39-6 CAPLUS

CN Thiocyanic acid, (1R,3aR,4R,5S,6R,7aS)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



SOURCE:

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:680627 CAPLUS

DOCUMENT NUMBER: 134:56805

TITLE: Enantiospecific total synthesis of both enantiomers of

2-thiocyanatoneopupukeanane from (R)-carvone

AUTHOR(S): Srikrishna, A.; Gharpure, Santosh J.

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of

Science, Bangalore, 560 012, India Perkin 1 (2000), (19), 3191-3193

CODEN: PERKF9; ISSN: 1470-4358
PUBLISHER: Royal Society of Chemistry

PUBLISHER: Royal Socie
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:56805

AB Enantiospecific synthesis of both enantiomers of the marine sesquiterpene 2-thiocyanatoneopupukeanane starting from (R)-carvone, employing an intramol. rhodium carbenoid C-H insertion reaction as the key step, is described.

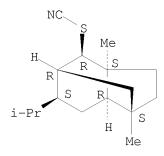
IT 137371-79-0P 313672-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of both enantiomers of 2-thiocyanatoneopupukeanane from (R)-carvone)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S,3aS,4R,5R,6S,7aR)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

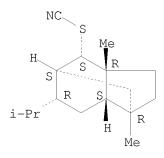
Absolute stereochemistry. Rotation (-).



RN 313672-32-1 CAPLUS

CN Thiocyanic acid, (1R, 3aR, 4S, 5S, 6R, 7aS) -octahydro-1, 3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:208836 CAPLUS

DOCUMENT NUMBER: 132:347746

TITLE: Bicentral bimolecular nucleophilic substitution (SN2)

in 2-methyl-1-chlorothioalkanes. Ab initio

calculations

AUTHOR(S): Apollonova, S. A.; Yermolaeva, L. V.; Plemenkov, V.

V.; Konovalov, A. I.

CORPORATE SOURCE: Kazan State Medical University, Kazan, Russia

SOURCE: Russian Journal of Organic Chemistry (Translation of

Zhurnal Organicheskoi Khimii) (1999), 35(8),

1135-1140

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

AB
AM1 and ab initio MO calcns. using the 3-21G(+) basis set for the mechanism of nucleophilic substitution in 2-(methylthio)-1-chloroethanes (I) and 4-mercapto-3-chlorocarane showed that the reaction with a cyanide anion occurs as 2 consecutives SN2 reactions which result in a product with reversed configuration at 2 reaction centers and with sulfide group transferred to the β -C atom. Both reactions have a common intermediate, a cyclic anion of thiirane structure containing both the attacking and leaving groups. A possibility of bicentral bimol. nucleophilic substitution (2-SN2) in I when the nucleophile attacks the α -C atom and the anion leaves the β -C atom was theor. shown for the 1st time.

IT 269065-17-0P

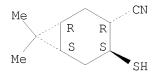
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(ab initio calcns. of bicentral bimol. nucleophilic substitution in 2-methyl-1-chlorothioalkanes)

RN 269065-17-0 CAPLUS

CN Bicyclo[4.1.0]heptane-3-carbonitrile, 4-mercapto-7,7-dimethyl-, (1R,3R,4S,6S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:495688 CAPLUS

DOCUMENT NUMBER: 129:214362

TITLE: Thiocyanate biosynthesis in the tropical marine sponge

Axinyssa n.sp.

AUTHOR(S): Simpson, Jamie S.; Garson, Mary J.

CORPORATE SOURCE: Department of Chemistry, The University of Queensland,

Brisbane, QLD 4072, Australia

SOURCE: Tetrahedron Letters (1998), 39(32),

5819-5822

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB The biosynthetic origin of the thiocyanate carbon in 2-

thiocyanatoneopupukeanane is defined by incorporation of sodium [14C] cyanide and [14C] thiocyanate into Axinyssa n.sp. The specificity of

incorporation is demonstrated by reduction of 2-thiocyanatoneopupukeanane to the thiol.

IT 137371-79-0P 212510-85-5P

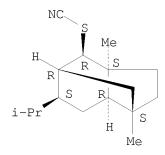
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)

(thiocyanate biosynthesis in the tropical marine sponge Axinyssa)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S,3aS,4R,5R,6S,7aR)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

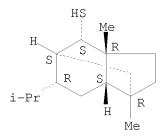
Absolute stereochemistry. Rotation (-).



RN 212510-85-5 CAPLUS

CN 1,5-Methano-1H-indene-8-thiol, octahydro-1,3a-dimethyl-6-(1-methylethyl)-, (1R,3aR,5S,6R,7aS,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:411000 CAPLUS

DOCUMENT NUMBER: 129:15921

TITLE: Photochemistry of Aliphatic Thioketones in the Gas

Phase

AUTHOR(S): Morrison, Harry; Lu, Yuelie; Carlson, Dean

CORPORATE SOURCE: Department of Chemistry, Purdue University, West

Lafayette, IN, 47907-1393, USA

SOURCE: Journal of Physical Chemistry A (1998),

102(28), 5421-5432

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:15921

vibrationally excited levels of S2.

The solution and gas-phase photophys. and photochem. properties of a series of bicyclic and alicyclic thioketones, i.e. apothiocamphor, thiocamphor, thiofenchone, endo-5,6-trimethylene-2-norbornanethione, 3,3-diethylbicyclo[3.2.1]octane-2-thione, 2,2-diethyl-5,5-dimethylcyclopentanethione, 2-ethyl-2,6,6-trimethylcyclohexanethione, and 2,4,4-trimethyl-3-hexanethione, were reported. Photolysis in solution typically gave products arising from insertion into β , γ , and, in the one case of endo-5,6-trimethylene-2-norbornanethione, δ carbons to form cyclic thiols. This chemical was analogous to that observed in earlier studies. Novel photochem. was found in the gas phase where Norrish type II products were also isolated from several substrates. The effect of the quencher gas, butane, on both the spectral and photochem. properties of thiocamphor in the gas phase provide evidence to support the

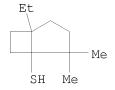
IT 205485-93-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (photochem. and spectral properties of aliphatic thicketones in the gas phase)

proposal that the Norrish type II chemical arises from initially populated

RN 205485-93-4 CAPLUS

CN Bicyclo[3.2.0]heptane-1-thiol, 5-ethyl-2,2-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:111981 CAPLUS

DOCUMENT NUMBER: 128:241934

TITLE: Terpene metabolites from the tropical marine sponge

Axinyssa sp. nov

AUTHOR(S): Simpson, Jamie S.; Garson, Mary J.; Hooper, John N.

A.; Cline, Edith I.; Angerhofer, Cindy K.

CORPORATE SOURCE: Department of Chemistry, The University of Queensland,

Brisbane, QLD. 4072, Australia

SOURCE: Australian Journal of Chemistry (1997),

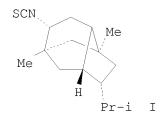
50(12), 1123-1127

CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER: CSIRO Australia

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ



AB A new sesquiterpene isothiocyanate, (-)-9-isothiocyanatopupukeanane (I), has been isolated along with the known sesquiterpene metabolites

(-) -9-isocyanopupukeanane, (-) -2-thiocyanatoneopupukeanane and

(-)-epipolasin-A from the sponge Axinyssa sp. nov. Three metabolites showed modest in vitro antimalarial activity.

IT 137371-79-0P

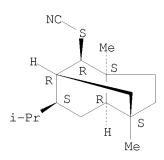
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(terpene metabolites isolation and structural characterization and antimalarial and cytotoxic activity from marine sponge Axinyssa)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S,3aS,4R,5R,6S,7aR)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:433913 CAPLUS

DOCUMENT NUMBER: 125:110580

TITLE: New antifouling sesquiterpenes from four nudibranchs

of the family Phyllidiidae

AUTHOR(S): Okino, Tatsufumi; Yoshimura, Erina; Hirota, Hiroshi;

Fusetani, Nobuhiro

CORPORATE SOURCE: Res. Dev. Corp. Japan, Niigata Eng. Co., Ltd.,

Yokohama, 235, Japan

SOURCE: Tetrahedron (1996), 52(28), 9447-9454

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier

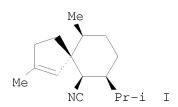
DOCUMENT TYPE:

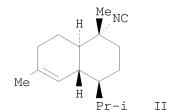
LANGUAGE:

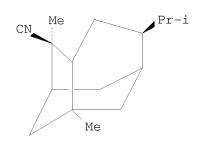
Journal English

III

GΙ







Me O Pr-i IV

AB Three new antifouling sesquiterpene isocyanides (I-III) were isolated from nudibranchs of the family Phyllidiidae along with a new sesquiterpene peroxide (IV) and 6 known sesquiterpenes. Their structures were determined mainly on the basis of 2-dimensional NMR data. These compds. showed potent antifouling activity against larvae of the barnacle Balanus amphitrite.

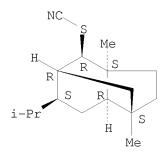
IT 137371-79-0

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S,3aS,4R,5R,6S,7aR)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:423807 CAPLUS

DOCUMENT NUMBER: 125:160835

TITLE: Antifouling activity of isocyanoterpenoids and related

compounds isolated from a marine sponge and

Nudibranchs

AUTHOR(S): Fusetani, Nobuhiro; Hiroto, Hiroshi; Okino, Tatsufumi;

Tomono, Yasuhiko; Yoshimura, Erina

CORPORATE SOURCE: Graduate School Agriculture and Agricultural Life

Science, University Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Natural Toxins (1996), 5(2),

249-259

CODEN: JNTOER; ISSN: 1058-8108

PUBLISHER: Alaken
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A total of 32 sesquiterpenes and diterpenes comprising isocyano, isothiocyano, or related functionalities were isolated as antifouling agents against cyprid larvae of the barnacle Balanus amphitrite from the marine sponge Acanthella cavernosa and three species of nudibranchs of the family Phyllidiidae. Several isocyanoterpenoids, e.g., kalihinol A, 10-formamidokalihinene, 15-formamidokalihinene, 13-isocyanotheonellin, and 10-isocyano-4-cadinene were highly antifouling, whereas their toxicity to cyprids were quite low. These results suggested that marine isocyanoterpenes are promising antifouling agents.

IT 137371-79-0

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

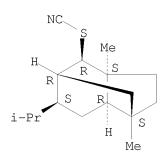
(antifouling activity of isocyanoterpenoids and related compds.

isolated from a marine sponge and Nudibranchs)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S, 3aS, 4R, 5R, 6S, 7aR) -octahydro-1, 3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:382346 CAPLUS

DOCUMENT NUMBER: 125:114866

TITLE: Synthesis of carane sulfide derivatives by reaction of

3-carene sulfides with functional derivatives of

mercaptans

AUTHOR(S): Fedyunina, I. V.; Plemenkov, V. V.; Nikitina, L. E.;

Litvinov, I. A.; Kataeva, O. N.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, Russia SOURCE: Khimiya Prirodnykh Soedinenii (1995), (4),

576-580

CODEN: KPSUAR; ISSN: 0023-1150

PUBLISHER: Fan
DOCUMENT TYPE: Journal
LANGUAGE: Russian

GΙ

AB Reaction of 3-carene α - and β -sulfide with 2-mercaptoethanol gave isomers of 4-[(2-hydroxyethyl)thio]-3-caranethiol and 3-[(2-hydroxyethyl)dithio]-4-[(2-hydroxyethyl)thio]carane. Reaction of the β -episulfide with mercaptoacetic acid gave heterocycle I.

IT 179032-44-1P 179032-45-2P 179237-36-6P 179237-37-7P

Ι

RN 179032-44-1 CAPLUS

CN Ethanol, 2-[(4-mercapto-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-, [1R-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 179032-45-2 CAPLUS

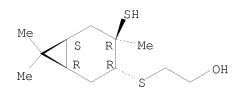
CN Ethanol, 2-[[4-[(2-hydroxyethyl)dithio]-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl]thio]-, [1S-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 179237-36-6 CAPLUS

CN Ethanol, 2-[(4-mercapto-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-, [1R-(1α , 3α , 4β , 6α)]- (9CI) (CA INDEX NAME)

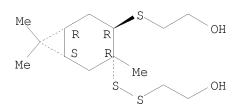
Absolute stereochemistry.



RN 179237-37-7 CAPLUS

CN Ethanol, 2-[[4-[(2-hydroxyethyl)thio]-3,7,7-trimethylbicyclo[4.1.0]hept-3-yl]dithio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:169716 CAPLUS

DOCUMENT NUMBER: 124:317492

TITLE: A new practical synthesis of (+)-grandisol from

(+)-citronellol using an intramolecular carbenoid

cyclization

AUTHOR(S): Monteiro, Hugo J.; Zukerman-Schpector, Julio

CORPORATE SOURCE: Dep. Quimica, Univ. Brasilia, Brasilia, 70910-900,

Brazil

SOURCE: Tetrahedron (1996), 52(11), 3879-88

CODEN: TETRAB; ISSN: 0040-4020

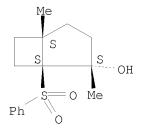
PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:317492

AB A new practical 10 step synthesis of (1S,2R)-2-acetyl-1-

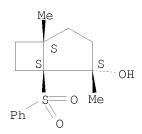
methylcyclobutaneacetic acid (I) is reported, which has a key step a rhodium catalyzed intramol. carbenoid cyclization of the α -diazo- β -ketosulfone, R-PhSO2C(:N2)COCH2CH2CHMeCH2CH2OMe, readily available from (+)-citronellol. Since I has already been converted into (+)-grandisol, the major pheromone of the cotton boll-weevil Anthonomus grandis, the described preparation constitutes a new formal synthesis of he optically active pheromone. 175882-22-1P 176021-13-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of (+)-grandisol from (+)-citronellol using intramol. carbenoid cyclization) RN 175882-22-1 CAPLUS CN Bicyclo[3.2.0]heptan-2-ol, 2,5-dimethyl-1-(phenylsulfonyl)-, $[1S-(1\alpha, 2\beta, 5\alpha)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 176021-13-9 CAPLUS CN Bicyclo[3.2.0]heptan-2-ol, 2,5-dimethyl-1-(phenylsulfonyl)-, $(1\alpha, 2\beta, 5\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:821294 CAPLUS

DOCUMENT NUMBER: 123:340410

TITLE: Synthesis of caranoids with two sulfide groups from

 $\alpha\text{--}$ and $\beta\text{--}thiooxide of 3-carene$

AUTHOR(S): Fedyunina, I. V.; Nikitina, L. E.; Plemenkov, V. V.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, Russia SOURCE: Khimiya Prirodnykh Soedinenii (1993), (5),

677-84

CODEN: KPSUAR; ISSN: 0023-1150

PUBLISHER: Fan
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Reaction of carene epoxides with thiourea hemisulfate gave the episulfides. Addition of Na thiolates to the episulfides gave

4-(alkylthio)-3-caranethiols, which were then alkylated on the SH group.

IT 170509-55-4P 170509-56-5P 170509-57-6P 170509-58-7P 170509-59-8P 170509-60-1P 170509-61-2P 170509-62-3P 170509-63-4P 170509-64-5P 170509-65-6P 170716-52-6P 170716-53-7P 170716-54-8P 170716-55-9P

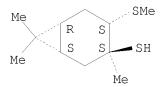
170716-53-7P 170716-54-8P 170716-53-9P 170716-58-2P

170897-50-4P

RN 170509-55-4 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-(methylthio)-, [1S- $(1\alpha, 3\alpha, 4\beta, 6\alpha)$]- (9CI) (CA INDEX NAME)

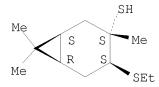
Absolute stereochemistry. Rotation (+).



RN 170509-56-5 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 4-(ethylthio)-3,7,7-trimethyl-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

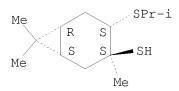
Absolute stereochemistry. Rotation (+).



RN 170509-57-6 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-[(1-methylethyl)thio]-, [1S-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



10/923,271

RN 170509-58-7 CAPLUS

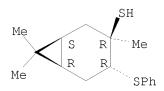
CN Bicyclo[4.1.0]heptane-3-thiol, 4-(butylthio)-3,7,7-trimethyl-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 170509-59-8 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-(phenylthio)-, (1S,3R,4R,6R)- (CA INDEX NAME)

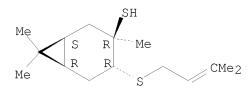
Absolute stereochemistry.



RN 170509-60-1 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-[(3-methyl-2-butenyl)thio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170509-61-2 CAPLUS

CN Disulfide, bis[3,7,7-trimethyl-4-[(3-methyl-2-butenyl)thio]bicyclo[4.1.0]hept-3-yl], [1S-[1 α ,3 β (1R*,3S*,4S*,6S*),4 α ,6 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170509-62-3 CAPLUS

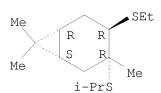
CN Bicyclo[4.1.0]heptane, 4-(ethylthio)-3,7,7-trimethyl-3-(methylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170509-63-4 CAPLUS

CN Bicyclo[4.1.0]heptane, 4-(ethylthio)-3,7,7-trimethyl-3-[(1-methylethyl)thio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170509-64-5 CAPLUS

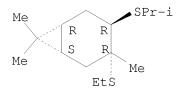
CN Bicyclo[4.1.0]heptane, 4-(ethylthio)-3,7,7-trimethyl-3-[(3-methyl-2-butenyl)thio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170509-65-6 CAPLUS

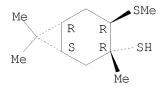
CN Bicyclo[4.1.0]heptane, 3-(ethylthio)-3,7,7-trimethyl-4-[(1-methylethyl)thio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170716-52-6 CAPLUS
CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-(methylthio)-, (1S,3R,4R,6R)- (CA INDEX NAME)

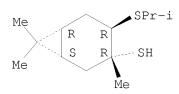
Absolute stereochemistry. Rotation (-).



RN 170716-53-7 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 3,7,7-trimethyl-4-[(1-methylethyl)thio]-, $(1\alpha, 3\beta, 4\alpha, 6\alpha)$ - (9CI) (CA INDEX NAME)

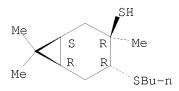
Absolute stereochemistry. Rotation (-).



RN 170716-54-8 CAPLUS

CN Bicyclo[4.1.0]heptane-3-thiol, 4-(butylthio)-3,7,7-trimethyl-, (1S,3R,4R,6R)- (CA INDEX NAME)

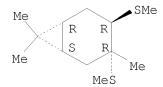
Absolute stereochemistry. Rotation (-).



RN 170716-55-9 CAPLUS

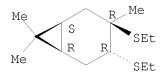
CN Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-3,4-bis(methylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



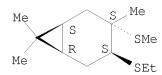
RN 170716-56-0 CAPLUS CN Bicyclo[4.1.0]heptane, 3,4-bis(ethylthio)-3,7,7-trimethyl-, [1S- $(1\alpha, 3\beta, 4\alpha, 6\alpha)$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



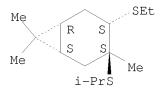
RN 170716-57-1 CAPLUS CN Bicyclo[4.1.0]heptane, 4-(ethylthio)-3,7,7-trimethyl-3-(methylthio)-, $(1\alpha,3\alpha,4\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



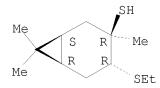
RN 170716-58-2 CAPLUS CN Bicyclo[4.1.0]heptane, 4-(ethylthio)-3,7,7-trimethyl-3-[(1-methylethyl)thio]-, $(1\alpha,3\alpha,4\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170897-50-4 CAPLUS CN Bicyclo[4.1.0]heptane-3-thiol, 4-(ethylthio)-3,7,7-trimethyl-, (1S,3R,4R,6R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:8529 CAPLUS

DOCUMENT NUMBER: 120:8529

ORIGINAL REFERENCE NO.: 120:1877a,1880a

TITLE: Reaction of 3,3-disubstituted cyclopropenes and other

cycloolefins with 1-phenyltetrazole-5-sulfenyl

chloride

AUTHOR(S): Khaliullin, R. R.; Plemenkov, V. V.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, Russia

SOURCE: Zhurnal Obshchei Khimii (1993), 63(4), 874-9

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 120:8529

AB The title reaction, including 3-carene, gave 2-chloro-1-(1-phenyltetrazolylthio)cycloalkanes. The stereoselectivity of

heterylphenylsulfenyl chloride addition to unsym. 3,3-disubstituted cyclopropenes was determined both by orbital and by steric factors. The

reaction may be used as a convenient method for introduction of a

heterocyclic group into the functional environment of a cyclopropane ring.

IT 94268-56-1P 151693-43-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 94268-56-1 CAPLUS

CN Bicyclo[4.1.0]hept-3-ene-3-thiol, 4,7,7-trimethyl- (CA INDEX NAME)



RN 151693-43-5 CAPLUS

CN 1H-Tetrazole, 5-[(4-chloro-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-1-phenyl- (CA INDEX NAME)

L4 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:487084 CAPLUS

DOCUMENT NUMBER: 117:87084

ORIGINAL REFERENCE NO.: 117:15131a, 15134a

TITLE: Sesquiterpene thiocyanates and isothiocyanates from

Axinyssa aplysinoides

AUTHOR(S): He, Hai Yin; Salva, Javier; Catalos, Robert F.;

Faulkner, D. John

CORPORATE SOURCE: Scripps Inst. Oceanogr., Univ. California, San Diego,

La Jolla, CA, 92093-0212, USA

SOURCE: Journal of Organic Chemistry (1992), 57(11),

3191 - 4

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

AB A specimen of Axinyssa (= Trachyopsis) aplysinoides from Palau contains (1R*,2R*,3R*,5R*,6S*,7S*)-2-thiocyanatopupukeanane. A specimen of A. aplysinoides from Pohnpei yielded two new isothiocyanates, (1S*,2R*,5S*,6S*,7R*,8S)-13-isothiocyanatocubebane and (1R*,4S*,5R*,6S*,7S*,10R*)-1-isothiocyanatoaromadendrane. A second specimen of A. aplysinoides from Pohnpei contained axisonitrile-3 and (1S*,2S*,3R*,6R*,7S*,9R*)-2-thiocyanatoneopupukaenane, which has a different stereochem. at C-2 to that assigned previously.

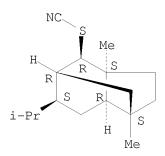
IT 137371-79-0

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
BIOL (Biological study); OCCU (Occurrence)
 (of sponge)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S, 3aS, 4R, 5R, 6S, 7aR) -octahydro-1, 3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:129272 CAPLUS

DOCUMENT NUMBER: 116:129272

ORIGINAL REFERENCE NO.: 116:21903a,21906a

TITLE: Synthesis of sulfide derivatives of the carane series

by reaction of 3-carene oxide with Functional

mercaptans

AUTHOR(S): Artemova, N. P.; Bikbulatova, G. Sh.; Plemenkov, V.

V.; Naumov, V. A.; Kataeva, O. N.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR

SOURCE: Khimiya Prirodnykh Soedinenii (1991), (2),

193-8

CODEN: KPSUAR; ISSN: 0023-1150

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 116:129272

GΙ

AB Reaction of 3-carene epoxide (I) with mercaptans under base-catalyzed conditions proceeds regio- and stereoselectively, and is a convenient process for obtaining polyfunctional 3-carene derivs. and products of their chemical transformations, e.g. hydroxyethylthiocaranols, alkylthiocaranolcarboxylates, and carane thiolactones. A new type of bicyclic terpene, bis(hydroxycaranyl) sulfides, is obtained together with the above products. Thus, treating I with HSCH2CO2H in EtOH containing NaOEt gave 16% carboxylic acid II and 9% sulfide III. Heating II in H2O at 90° gave 20.5% spiro derivative IV.

IT 139259-48-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of, thiolactone from)

RN 139259-48-6 CAPLUS

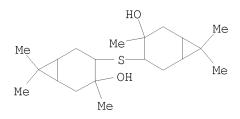
CN Acetic acid, [(4-hydroxy-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-,

 $[1R-(1\alpha, 3\beta, 4\alpha, 6\alpha)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 135028-46-5 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, [1S-[1 α ,3 α ,4 β (1'R*,3'R*,4'R*,6'S*),6 α]]- (9CI) (CA INDEX NAME)



RN 135028-49-8 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, [1S-[1 α ,3 β ,4 α (1'R*,3'S*,4'S*,6'S*),6 α]]- (9CI) (CA INDEX NAME)

RN 139259-47-5 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4-[(2-hydroxyethyl)thio]-3,7,7-trimethyl-, [1S-(1α , 3α , 4β , 6α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139259-50-0 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4-[(2-hydroxyethyl)thio]-3,7,7-trimethyl-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139259-51-1 CAPLUS

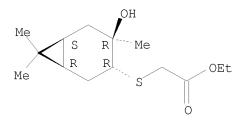
CN Acetic acid, [(4-hydroxy-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-, [1R-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139259-53-3 CAPLUS

CN Acetic acid, [(4-hydroxy-4,7,7-trimethylbicyclo[4.1.0]hept-3-yl)thio]-, ethyl ester, [1R-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:41777 CAPLUS

10/923,271

DOCUMENT NUMBER: 116:41777

ORIGINAL REFERENCE NO.: 116:7185a,7188a

TITLE: Reaction of 3-carene oxides with thiourea

AUTHOR(S): Artemova, N. P.; Bikbulatova, G. Sh.; Plemenkov, V.

V.; Efremov, Yu. Ya.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR SOURCE: Zhurnal Obshchei Khimii (1991), 61(6),

1484-5

CODEN: ZOKHA4; ISSN: 0044-460X

ΙI

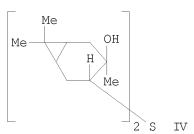
DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 116:41777

GΙ

Me Me Me Me CH₂S

Me Me Me S III



AB Reaction of 3-carene epoxides I with thiourea in EtOH gave disulfide II. When EtONa was added to reaction the sulfides III and IV were formed.

IT 138232-97-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, via reaction of carene α -epoxide with thiourea and ethoxide)

RN 138232-97-0 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, $[1\alpha,3\alpha,4\beta(1'R^*,3'R^*,4'R^*,6'S^*),6\alpha]$ - (9CI) (CA INDEX NAME)

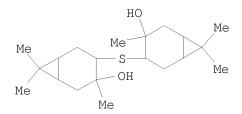
Me Me Me Me Me Me

IT 138232-98-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, via reaction of carene β -epoxide with thiourea and ethoxide)

RN 138232-98-1 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, [2α , 3β , 4α (1'R*,3'S*,4'S*,6'S*), 6α]- (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:652363 CAPLUS

DOCUMENT NUMBER: 115:252363

ORIGINAL REFERENCE NO.: 115:42817a,42820a

TITLE: Two marine sesquiterpene thiocyanates

AUTHOR(S): Pham, Anthony T.; Ichiba, Toshio; Yoshida, Wesley Y.;

Scheuer, Paul J.; Uchida, Tomohiro; Tanaka, Junichi;

Higa, Tatsuo

CORPORATE SOURCE: Dep. Chem., Univ. Hawaii, Manoa, Honolulu, HI, 96822,

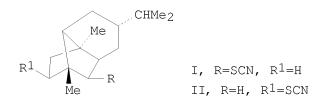
USA

SOURCE: Tetrahedron Letters (1991), 32(37), 4843-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ



AB From two sponges collected in Pohnpei (unidentified) and Okinawa (Phycopsis terpnis) 2-(I) and 4-thiocyanatoneopupukeanane (II) were isolated.

IT 137371-79-0

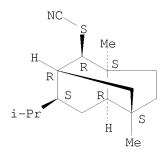
RL: PROC (Process)

(isolation of, from marine sponge)

RN 137371-79-0 CAPLUS

CN Thiocyanic acid, (1S,3aS,4R,5R,6S,7aR)-octahydro-1,3a-dimethyl-6-(1-methylethyl)-1,5-methano-1H-inden-4-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:471910 CAPLUS

DOCUMENT NUMBER: 115:71910

ORIGINAL REFERENCE NO.: 115:12443a,12446a

TITLE: Reactions of 3-carene oxides with allyl- and

benzylisothiouronium salts

AUTHOR(S): Artemova, N. P.; Bikbulatova, G. Sh.; Plemenkov, V.

V.; Litvinov, I. A.; Kataeva, O. N.; Surkova, L. N.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR

SOURCE: Zhurnal Obshchei Khimii (1990), 60(10),

2374-81

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 115:71910

GΙ

AB The reaction of α - and β -3,4-epoxycaranes with RSC(:NH)NH2.HX (R = allyl, X = Br; R = PhCH2, X = Cl) in EtOH-NaOEt proceeds stereo- and regioselectively to give caranols I and II, resp. in addition to bis(3-hydroxy-4-caranyl)sulfides III and IV.

IT 135028-46-5P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure of) RN 135028-46-5 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, [1S-[1 α ,3 α ,4 β (1'R*,3'R*,4'R*,6'S*),6 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 134927-26-7 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(phenylmethyl)thio]-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

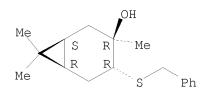
RN 135028-47-6 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(2-propenylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 135028-48-7 CAPLUS

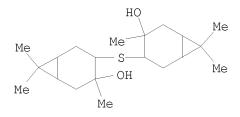
CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(phenylmethyl)thio]-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 135028-49-8 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4,4'-thiobis[3,7,7-trimethyl-, [1S-[1 α ,3 β ,4 α (1'R*,3'S*,4'S*,6'S*),6 α]]- (9CI) (CA INDEX NAME)



L4 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:471909 CAPLUS

DOCUMENT NUMBER: 115:71909

ORIGINAL REFERENCE NO.: 115:12443a,12446a

TITLE: Lewis acid catalyzed addition of disulfides to

3-carene

AUTHOR(S): Nikitina, L. E.; Plemenkov, V. V.; Chernov, A. N.;

Litvinov, I. A.; Kataeva, O. N.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR SOURCE: Zhurnal Obshchei Khimii (1990), 60(10),

2303-8

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Reaction of 3-carene with R2S2 (R = Me, Et) in the presence of ZnCl2 is a convenient method for obtaining S-containing derivs. of carane with two alkythio groups and alkylsulfonyl groups at the C3 and C4 carbons. Ph2S2 in this reaction gives 4-phenylthiocarene. The addition takes place

trans-stereoselectively with electrophilic attack at the position trans to the cyclopropane fragment. The sensitivity of the process to steric factors contributes to the low yields of products of cis-addition and to formal substitution products.

IT 134927-33-6P

RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in reaction of carene with di-Ph disulfide)

RN 134927-33-6 CAPLUS

CN Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-4-(phenylthio)- (CA INDEX NAME)



IT 134927-27-8P 134927-28-9P 134927-30-3P 134927-31-4P

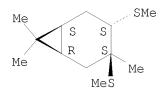
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 134927-27-8 CAPLUS

CN Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-3,4-bis(methylthio)-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

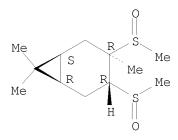
Relative stereochemistry.



RN 134927-28-9 CAPLUS

CN Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-3,4-bis(methylsulfinyl)-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

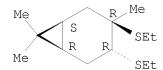
Relative stereochemistry.



RN 134927-30-3 CAPLUS

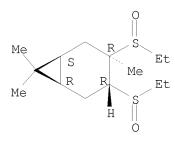
CN Bicyclo[4.1.0]heptane, 3,4-bis(ethylthio)-3,7,7-trimethyl-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

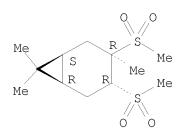


RN 134927-31-4 CAPLUS CN Bicyclo[4.1.0]heptane, 3,4-bis(ethylsulfinyl)-3,7,7-trimethyl-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

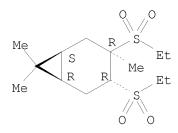


Relative stereochemistry.



RN 134927-32-5 CAPLUS CN Bicyclo[4.1.0]heptane, 3,4-bis(ethylsulfonyl)-3,7,7-trimethyl-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

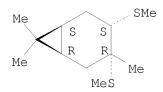
Relative stereochemistry.



RN 135028-50-1 CAPLUS

CN Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-3,4-bis(methylthio)-, $(1\alpha,3\alpha,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

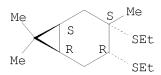
Relative stereochemistry.



RN 135028-51-2 CAPLUS

CN Bicyclo[4.1.0]heptane, 3,4-bis(ethylthio)-3,7,7-trimethyl-, $(1\alpha,3\alpha,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:143721 CAPLUS

DOCUMENT NUMBER: 114:143721

ORIGINAL REFERENCE NO.: 114:24401a,24404a

TITLE: Reactions of 3-carene oxides with isothiuronium salts.

Synthesis and molecular structure of 4-alkylthio- and

4-alkylsulfonylcaran-3-ols

AUTHOR(S): Artemova, N. P.; Bikbulatova, G. Sh.; Plemenkov, V.

V.; Litvinov, I. A.; Kataeva, O. N.; Naumov, V. A.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR SOURCE: Zhurnal Obshchei Khimii (1989), 59(12),

2718-24

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 114:143721

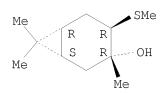
GI

AB cis- And trans-3,4-epoxycaranes react with RSC(:NH)NH2.HX (R = Me, X = sulfate; R = Et, X = Br; R = Me2CH, X = iodide) regio- and stereoselectively to give alkylthiocaranols I from trans-reactant and II from cis-reactant. Oxidation of I and II by H2O2 gives the corresponding sulfones.

RN 98796-82-8 CAPLUS

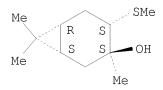
CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127181-77-5 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylthio)-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

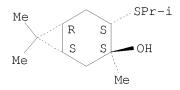


RN 127181-78-6 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4-(ethylthio)-3,7,7-trimethyl-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

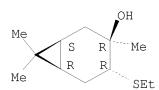
RN 127181-79-7 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(1-methylethyl)thio]-, $[1S-(1\alpha,3\alpha,4\beta,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



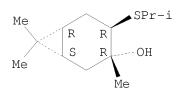
RN 127181-80-0 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4-(ethylthio)-3,7,7-trimethyl-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



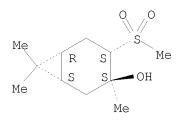
RN 127181-81-1 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(1-methylethyl)thio]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



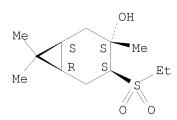
[1S-
$$(1\alpha, 3\alpha, 4\beta, 6\alpha)$$
]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



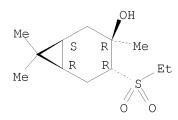
RN 127118-69-8 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4-(ethylsulfonyl)-3,7,7-trimethyl-, [1S-(1
$$\alpha$$
,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127181-82-2 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 4-(ethylsulfonyl)-3,7,7-trimethyl-, [1S-(1
$$\alpha$$
,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127182-21-2 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylsulfonyl)-, [1S-(1
$$\alpha$$
,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

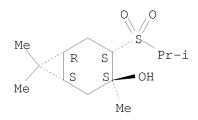
IT 127118-70-1P 127181-83-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, crystal structure, and mol. structure of)

RN 127118-70-1 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(1-methylethyl)sulfonyl]-, [1S-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

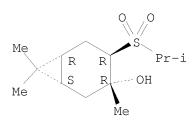
Absolute stereochemistry.



RN 127181-83-3 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(1-methylethyl)sulfonyl]-, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:121541 CAPLUS

DOCUMENT NUMBER: 114:121541

ORIGINAL REFERENCE NO.: 114:20693a,20696a

TITLE: Rearrangements of 1,4,4- and 2,2,5- trimethylbicyclo[3.2.1]oct-6-yl cations

AUTHOR(S): Kirmse, Wolfgang; Moench, Dietmar

CORPORATE SOURCE: Fak. Chem., Ruhr-Univ. Bochum, Bochum, D-4630/1,

Germany

SOURCE: Chemische Berichte (1991), 124(1), 237-40

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:121541
GI For diagram(s), see printed CA Issue.

1,4,4-Trimethylbicyclo[3.2.1]oct-6-yl cations (I) are generated from the AB tosylhydrazone (RR1 = NNHTs), by nitrous acid deamination of the amines II (R = NH2, R1 = H; R = H, R1 = NH2) and by acetolysis of the brosylates II (R = D, R1 - OBs; R = OBs, R1 = O). The product distributions are but slightly affected by the configuration (exo vs. endo) of the leaving groups. The predominant product, 1,4,4-trimethylbicyclo[3.2.1]octan-exo-6ol (II, R = OH, R1 = H) is formed without significant redistribution of a 6-2H label. The degenerate Wagner-Meerwein rearrangement of the parent 6-bicyclo[3.2.1]octyl cation is virtually eliminated by the presence of two Me groups at C-4. Enhanced conformational strain, raising the barrier to ring flipping, accounts for these observations. Minor products arise from a 7,6-hydride shift of I, followed by Wagner-Meerwein rearrangement. When the 2,2,5-trimethylbicyclo[3.2.1]oct-6-yl cation III is generated directly from the tosylhydrazone IV, the tertiary alc. V is obtained as the major product. The conformational barrier to Wagner-Meerwein rearrangement is compensated by the incipient stabilization of the tertiary carbocation.

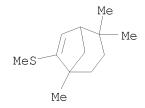
IT 130380-84-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 130380-84-6 CAPLUS

CN Bicyclo[3.2.1]oct-6-ene, 1,4,4-trimethyl-7-(methylthio)- (CA INDEX NAME)



L4 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:612355 CAPLUS

DOCUMENT NUMBER: 113:212355

ORIGINAL REFERENCE NO.: 113:35895a,35898a

TITLE: Nucleophilic substitution in β -

chloro(alkylthio) caranes obtained by electrophilic

chlorosulfenylation of 3-carene

AUTHOR(S): Plemenkov, V. V.; Bairamova, F. A.; Butenko, G. G.;

Artemova, N. P.; Litvinov, I. A.; Naumov, V. A.;

Il'yasov, A. V.; Udarov, B. G.

CORPORATE SOURCE: Kazan. Gos. Med. Inst., Kazan, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1990), 26(5),

1010-16

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 113:212355

GΙ

AB Treating 3-carene with RSCl (R = Me, Et, Ph) in Et20 gave 95-96% alkylthiocaranes I which (R = Me) was hydrolyzed by aqueous KOH to give 70% caranol II followed by oxidation to give the sulfone III. Heating I (R = Me) with Et4N+CN- gave 65% nitrile IV which was oxidized to the sulfone followed by desulfonylation with KOCMe3 to give 47% nitrile V.

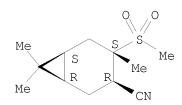
IT 130321-31-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and elimination of methylsulfenyl group from)

RN 130321-31-2 CAPLUS

CN Bicyclo[4.1.0]heptane-3-carbonitrile, 4,7,7-trimethyl-4-(methylsulfonyl)-, $(1\alpha, 3\beta, 4\alpha, 6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 130226-58-3P 130321-29-8P

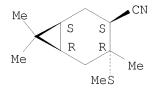
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 130226-58-3 CAPLUS

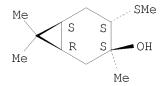
CN Bicyclo[4.1.0]heptane-3-carbonitrile, 4,7,7-trimethyl-4-(methylthio)-, $(1\alpha, 3\beta, 4\alpha, 6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

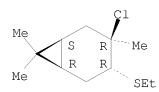


RN 130321-29-8 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylthio)-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

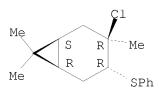


Relative stereochemistry.



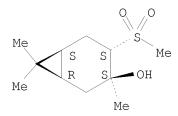
RN 130321-26-5 CAPLUS CN Bicyclo[4.1.0]heptane, 3-chloro-3,7,7-trimethyl-4-(phenylthio)-, $(1\alpha, 3\beta, 4\alpha, 6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 130321-30-1 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylsulfonyl)-, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



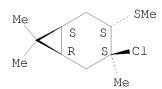
IT 130321-25-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, thermolysis, hydrolysis, and cyanation of)

RN 130321-25-4 CAPLUS

CN Bicyclo[4.1.0]heptane, 3-chloro-3,7,7-trimethyl-4-(methylthio)-, $(1\alpha, 3\beta, 4\alpha, 6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:506839 CAPLUS

DOCUMENT NUMBER: 113:106839

ORIGINAL REFERENCE NO.: 113:17907a,17910a

TITLE: Molecular structure and absolute configuration of

1(R), 3(S), 4(R), 6(R), 3, 7, 7-trimethyl-3-methylsulfonyl-4-

cyano-bicyclo[4.1.0]heptane

AUTHOR(S): Litvinov, I. A.; Naumov, V. A.; Plemenkov, V. V. CORPORATE SOURCE: Inst. Org. Fiz. Khim. im. Arbuzova, Kazan, USSR

SOURCE: Zhurnal Strukturnoi Khimii (1990), 31(2),

192-4

CODEN: ZSTKAI; ISSN: 0136-7463

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB The title compound is orthorhombic, space group P212121, with a 6.544(4), b

10.657(3), and c 18.410(6) Å; dc = 1.25 for Z = 4. The atomic

coordinates are given. The structure was solved by direct methods and refined by least-squares to R=0.032. The bond lengths and angles are

given. The absolute configuration is described.

IT 129085-28-5

RL: PRP (Properties)

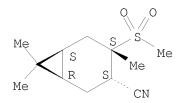
(absolute configuration and structure of)

RN 129085-28-5 CAPLUS

CN Bicyclo[4.1.0]heptane-3-carbonitrile, 4,7,7-trimethyl-4-(methylsulfonyl)-,

[1R- $(1\alpha, 3\alpha, 4\alpha, 6\alpha)$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:118322 CAPLUS

DOCUMENT NUMBER: 112:118322

ORIGINAL REFERENCE NO.: 112:20027a,20030a

TITLE: Method of producing 4β -(alkylthio)caran- 3α -

ols

INVENTOR(S): Plemenkov, V. V.; Bikbulatova, G. Sh.; Artemova, N.

P.; Surkova, L. N.; Il'yasov, A. V.; Nafikova, A. A.

PATENT ASSIGNEE(S): Kazakh State Medical Institute, USSR; Arbuzov, A. E.,

Institute of Organic and Physical Chemistry

SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1989, (29), 77-8.

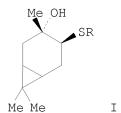
CODEN: URXXAF

DOCUMENT TYPE: Patent LANGUAGE: Russian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1498760	A1	19890807	SU 1987-4220849	19870331 <
PRIORITY APPLN. INFO.:			SU 1987-4220849	19870331
GI				



AB The title compds. (I; R = Et, Me2CH, Bu) are prepared by reaction of $\alpha-3,4-{\rm epoxycarane}$ with RSH in the presence of RSNa and Me2SO at $75-140\,^{\circ}.$

RN 85567-25-5 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4-(ethylthio)-3,7,7-trimethyl- (CA INDEX NAME)

RN 125600-35-3 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-[(1-methylethyl)thio]- (CA INDEX NAME)

RN 125600-36-4 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 4-(butylthio)-3,7,7-trimethyl- (CA INDEX NAME)

L4 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:595956 CAPLUS

DOCUMENT NUMBER: 103:195956

ORIGINAL REFERENCE NO.: 103:31569a,31572a

TITLE: On the chemistry of some [4.1.1] – and

[3.1.1]propellanes

AUTHOR(S):

Baumgart, Klaus Dieter; Harnisch, Hanna;
Szeimies-Seebach, Ursula; Szeimies, Guenter

CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2,

Fed. Rep. Ger.

SOURCE: Chemische Berichte (1985), 118(7), 2883-916

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 103:195956

GΙ

AB Thermal isomerization of propellanes e.g., I (R1 = H, Me, R2 = H), II or III gave 1,3-dienes IV-VI. The rates of these rearrangements were strongly enhanced by traces of unknown electrophilic reagents. Adding DABCO to the thermolysis solns. eliminated the rate accelerating effects. The intended rearrangement of the propellanes by electrophilic catalysts at room temperature proceeded with varying rates to give the expected dienes. However, using Me3SiCl and SiCl4 gave norcorenes, e.g. III gave VII. Also described were addition reactions and radical reactions of selected propellanes.

IT 98230-01-4P

RN 98230-01-4 CAPLUS

CN 12-Oxatetracyclo[7.2.1.02,7.03,8]dodecane, 2,10-bis(ethylthio)-1,9-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)

10/923,271

L4 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:578464 CAPLUS

DOCUMENT NUMBER: 103:178464

ORIGINAL REFERENCE NO.: 103:28731a,28734a

TITLE: Selective functionalization of (+)-3-carene

AUTHOR(S): Takabe, Kunihiko; Inamori, Masahito; Nashiki, Ryohei;

Yamada, Takashi; Katagiri, Takao

CORPORATE SOURCE: Dep. Synth. Chem., Shizuoka Univ., Hamamatsu, 432,

Japan

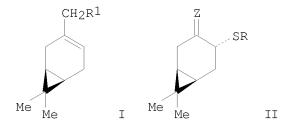
SOURCE: Shizuoka Daigaku Kogakubu Kenkyu Hokoku (1984

), 35, 25-9

CODEN: SDKKAT; ISSN: 0583-0915

DOCUMENT TYPE: Journal LANGUAGE: Japanese

GΙ



AB Regio- and stereoselective addition of RSCl (R = Ph, Me) to (+)-3-carene (I, R1 = H) gave 94-95% sulfide II (Z = α -Me, β -Cl), reaction of which with NaOAc/AcOH gave II (Z = α -Me, β -OAc). Dehydrochlorination or dehydration of II (Z = α -Me, β -Cl, β -OH) gave II (Z = CH2), thermal isomerization of which gave I (R1 = SR). I (R1 = Ph) is a key intermediate for the synthesis of natural products.

IT 91464-74-3P 98796-80-6P 98796-81-7P

98796-82-8P

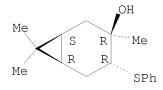
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of)

RN 91464-74-3 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 98796-80-6 CAPLUS

CN Bicyclo[4.1.0]heptane, 3-chloro-3,7,7-trimethyl-4-(phenylthio)-,

$$[1S-(1\alpha, 3\beta, 4\alpha, 6\alpha)]-(9CI)$$
 (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & C1 \\ & & & \\ S & & R \\ & R & R \\ & & \\ Me & & \\ SPh \end{array}$$

RN 98796-81-7 CAPLUS

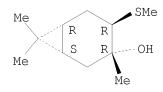
CN Bicyclo[4.1.0]heptane, 3-chloro-3,7,7-trimethyl-4-(methylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 98796-82-8 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

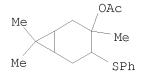
Absolute stereochemistry.



IT 91413-40-0P 98796-83-9P

RN 91413-40-0 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylthio)-, acetate, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)



RN 98796-83-9 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(methylthio)-, acetate, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-(9CI)$ (CA INDEX NAME)

L4 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:491246 CAPLUS

DOCUMENT NUMBER: 101:91246

ORIGINAL REFERENCE NO.: 101:13999a,14002a

TITLE: A facile route to (-)-car-4-en-3 α -ol and

(-)-car-4-en-3 β -ol, intermediates for bioactive synthetic pyrethroids, synthesis of tertiary allylic

alcohols by pyrolysis of sulfoxides

AUTHOR(S): Mitra, R. B.; Muljiani, Z.; Deshmukh, A. R. A. S.;

Joshi, V. S.; Gadre, S. R.

CORPORATE SOURCE: Natl. Chem. Lab., Poona City, 411 008, India

SOURCE: Synthetic Communications (1984), 14(2),

101-12

CODEN: SYNCAV; ISSN: 0039-7911

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

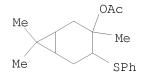
Me

AB (-)-Car-4-en-3 α -ol (I, R = OH, R1 = Me) and (-)-car-4-en-3 β -ol (I, R = Me, R1 = OH), intermediates for pyrethroids, were prepared via epoxidn. of (+)-3-carene (II) with H2O2, regio- and stereospecific

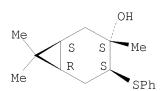
TOh 10/05/2008

IV

phenylsulfenylation of the resulting epoxide III with NaSPh, oxidation of the corresponding sulfides (IV, R-R2 = OH, Me, β -PhS; Me, OH, α -PhS; resp.) with H2O2, and pyrolysis of the corresponding sulfoxides [IV, R-R2 = OH, Me, PhS(O); Me, OH, α -PhS(O); resp.]. IT 91413-40-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)
RN 91413-40-0 CAPLUS
Sicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylthio)-, acetate, [1S-(1 α ,3 β ,4 α ,6 α)]- (9CI) (CA INDEX NAME)

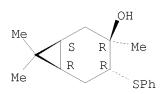


Absolute stereochemistry.



RN 91464-74-3 CAPLUS CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylthio)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

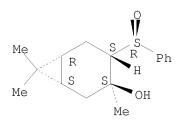
Absolute stereochemistry.



RN 91413-37-5 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylsulfinyl)-, $[1S-[1\alpha,3\alpha,4\beta(S^*),6\alpha]]$ - (9CI) (CA INDEX NAME)

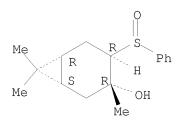
Absolute stereochemistry.



RN 91464-75-4 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylsulfinyl)-, $[1S-(1\alpha,3\beta,4\alpha,6\alpha)]-$ (9CI) (CA INDEX NAME)

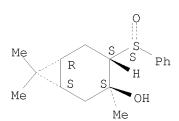
Absolute stereochemistry.



RN 91464-79-8 CAPLUS

CN Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-4-(phenylsulfinyl)-, $[1S-[1\alpha,3\alpha,4\beta(R^*),6\alpha]]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:203171 CAPLUS

DOCUMENT NUMBER: 90:203171

ORIGINAL REFERENCE NO.: 90:32309a,32312a

TITLE: On the stereochemistry of thiocarbonyl S2 hydrogen

abstraction

AUTHOR(S): Blackwell, D. S. L.; Lee, K. H.; De Mayo, P.;

Petrasiunas, G. L. R.; Reverdy, G.

CORPORATE SOURCE: Dep. Chem., Univ. Western Ontario, London, ON, Can.

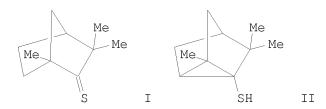
SOURCE: Nouveau Journal de Chimie (1979), 3(2),

123-31

CODEN: NJCHD4; ISSN: 0398-9836

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ



AB Excitation of bicyclic bridged alicyclic thiones into the S2 state gives intramol. cyclization and formation of cyclopropyl thiols (β -insertion). For example, irradiation of thiofenchone I gave thiol II. A study of the stereochem. leads to the conclusion that the volume of space active in the H abstraction and cyclization lies above and below the plane of the thiocarbonyl group. The reactive state is $(1\pi,\pi^*)$. The cyclopropyl thiols, on heating, revert to thiones, sometimes with rearranged C skeletons.

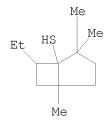
IT 70233-50-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 70233-50-0 CAPLUS

CN Bicyclo[3.2.0]heptane-1-thiol, 7-ethyl-2,2,5-trimethyl- (CA INDEX NAME)



L4 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:23329 CAPLUS

DOCUMENT NUMBER: 90:23329

ORIGINAL REFERENCE NO.: 90:3863a,3866a

TITLE: Terpene sulfides of ruthenium for resistors
INVENTOR(S): Komarov, V. P.; Lazarev, V. B.; Shaplygin, I. S.
PATENT ASSIGNEE(S): Kurnakov, N. S., Institute of General and Inorganic

Chemistry, USSR

SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,

Tovarnye Znaki 1978, 55(36), 102.

CODEN: URXXAF

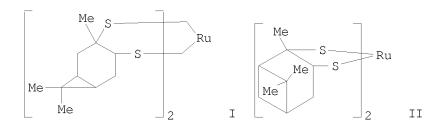
DOCUMENT TYPE: Patent Russian LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE _____ ____ _____ SU 626093 Α1 19780930 SU 1975-2175505 19750922 <--PRIORITY APPLN. INFO.: SU 1975-2175505 A 19750922

GΙ



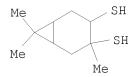
AΒ The title compds. I and II, were prepared by treating an alc. solution of Ru oxychloride or anhydrous RuCl3 with excess sulfurated turpentine, or dimercapto- $\Delta 3$ -carene or dimercaptopinene at 50-75°.

ΙT 68671-21-6

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with rutheium oxychloride and trichloride)

68671-21-6 CAPLUS RN

Bicyclo[4.1.0]heptane-3,4-dithiol, 3,7,7-trimethyl- (CA INDEX NAME) CN



ANSWER 33 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:556695 CAPLUS

DOCUMENT NUMBER: 89:156695

ORIGINAL REFERENCE NO.: 89:24155a,24158a

TITLE: Formation conditions and structure of gold terpene

sulfide

AUTHOR(S): Komarov, V. P.; Lazarev, V. B.

Inst. Obshch. Neorg. Khim. im. Kurnakova, Moscow, USSR CORPORATE SOURCE:

SOURCE: Zhurnal Neorganicheskoi Khimii (1978),

23(7), 1865-70 CODEN: ZNOKAQ; ISSN: 0044-457X

DOCUMENT TYPE: Journal LANGUAGE: Russian

GΙ

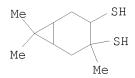
H₂L

AB The terpene dimercaptan (H2L) reacted with NH4AuCl4 to give Au2L which was characterized by IR and NMR spectra. H2L was obtained from the reaction of $\Delta 3$ -carene with S.

IT 67775-59-1P

RN 67775-59-1 CAPLUS

CN Bicyclo[4.1.0]heptane-3,4-dithiol, 3,7,7-trimethyl-, digold(1+) salt (9CI) (CA INDEX NAME)



●2 Au(I)

L4 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:442700 CAPLUS

DOCUMENT NUMBER: 79:42700

ORIGINAL REFERENCE NO.: 79:6945a,6948a

TITLE: Reaction of 3,4-epoxycaranes with sodium sulfite and

hydrogen sulfite

AUTHOR(S): Myslinski, Eugeniusz; Michalek, Emilia

CORPORATE SOURCE: N. Copernicus Univ., Torun, Pol. SOURCE: Roczniki Chemii (1973), 47(2), 285-9

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal LANGUAGE: Polish

GI For diagram(s), see printed CA Issue.

AB Trans-3,4-epoxycarane (I) treated with aqueous NaCHSO3 gave 52° of the alc. (II, R = OH). A similar reaction with cis-3,4-epoxycarane (III) yielded 61° of a 4:1 mixture of IV (R = OH) and diol V. When refluxed with an aqueous solution of Na2SO3, I gave after 85 hr 32° II (R = OH) and 27° of caranol IV (R = SO3Na). An analogous reaction

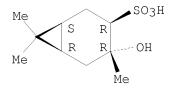
with III was complete in 245 hr, the major product (67°) being II (R = SO3Na), and the minor product (21°), a mixture of IV (Rf = OH) and V.

IT 43009-80-9P 43009-81-0P

RN 43009-80-9 CAPLUS

CN Bicyclo[4.1.0]heptane-3-sulfonic acid, 4-hydroxy-4,7,7-trimethyl-, monosodium salt, $(1\alpha,3\beta,4\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

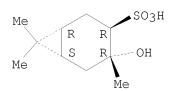


Na

RN 43009-81-0 CAPLUS

CN Bicyclo[4.1.0]heptane-3-sulfonic acid, 4-hydroxy-4,7,7-trimethyl-, monosodium salt, [1R-(1 α ,3 α ,4 β ,6 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Na

L4 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1964:9922 CAPLUS

DOCUMENT NUMBER: 60:9922 ORIGINAL REFERENCE NO.: 60:1798d-e

TITLE: Unsaturated thio alcohols of the carane series

AUTHOR(S): Myslinski, Eugeniusz; Krupowicz, Jan

CORPORATE SOURCE: Univ. Torun, Pol.

SOURCE: Roczniki Chemii (1963), 37(7/8), 787-94

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GΙ For diagram(s), see printed CA Issue. Hydrogenation of a mixture of carenyldithiocarenes with LiAlH4 yielded 13% AB d-3-carene, 55% I, b3 70-2°, d20 0.9873, n20D 1.5253, [α]20D 13.6°, and 28% II, b3 62-4°, d20 0.9671, n20D 1.5130, $[\alpha]$ 20D 91°. I and II desulfurized with Raney Ni gave the corresponding 3- or 4-carene. The infrared spectra of the products were examined 94268-56-1P, 3-Carene-4-thiol ΙT RL: PREP (Preparation) (preparation of) RN 94268-56-1 CAPLUS CN Bicyclo[4.1.0]hept-3-ene-3-thiol, 4,7,7-trimethyl- (CA INDEX NAME) Me Me Me SH ANSWER 36 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1963:435736 CAPLUS 59:35736 DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 59:6441b-d TITLE: Reaction of sulfur chloride with d-3-carene AUTHOR(S): Krupowicz, Jan; Myslinski, Eugeniusz CORPORATE SOURCE: Univ. Torun, Pol. SOURCE: Roczniki Chemii (1962), 36, 1575-81 CODEN: ROCHAC; ISSN: 0035-7677 DOCUMENT TYPE: Journal LANGUAGE: German GΙ For diagram(s), see printed CA Issue. SC12 (67.5 g.) was added during 4 hrs. at -5° , to a solution of 136 g. AB d-3-carene in 203.5 g. C6H6. The benzene solution, washed with saturated aqueous NaHCO3 and H2O and evaporated during 6 hrs. at 50° and 5 mm. Hq, gave 195 g. bis(4-chloro-3-caranyl) disulfide (I), n20D 1.5485, d20 1.1200,

 $[\alpha]20D$ -150.8° (C6H6). I, oxidized with KMnO4, afforded cis-caronic acid, m. 174-6°. I, dehydrochlorinated with C5H5N, gave a mixture of carenylodithiocarenes, n20D 1.5767, d20 1.1170, $[\alpha]$ 20D 132.4°, which, on desulfurization with Raney Ni, gave a mixture of d-3-carene and d-4-carene. Hydrogenation of the carene mixture with Adams catalyst in glacial AcOH afforded carane, b. 166-7°, n20D 1.4561, d20 0.8326, $[\alpha]$ 20D 2°, MRD 45.14. 99813-39-5P, Disulfide, bis(3-chloro-4-caryl) 104157-93-9P

ΙT , 3-Caren-4-vl disulfide RL: PREP (Preparation) (preparation of)

RN 99813-39-5 CAPLUS

Disulfide, bis(3-chloro-4-caryl) (7CI) (CA INDEX NAME) CN

RN 104157-93-9 CAPLUS

CN 3-Caren-4-yl disulfide (7CI) (CA INDEX NAME)

L4 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:436475 CAPLUS

DOCUMENT NUMBER: 57:36475
ORIGINAL REFERENCE NO.: 57:7313d-e

TITLE: Preparation of carene sulfoxide AUTHOR(S): Krupowicz, Jan; Wnek, Maria

CORPORATE SOURCE: Univ. Torun, Pol.

SOURCE: Roczniki Chemii (1961), 35, 1329-32

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Thionyl chloride (59 g.) was added dropwise 10 hrs. to 68 g. d-3-carene in the presence of 3 g. powdered Fe at -5° . The oil was dissolved in hot BuOH (I) and treated with aqueous NH3 to sep. the NH4 salts. Carene sulfoxide (II), m. 120° (decomposition), was precipitated from the filtrate by addition

200 ml. EtOH and must be recrystd. from I. The yield may be very small. Oxidation of II with KMnO4 gave cis-caronic acid, m. $170-1^{\circ}$.

IT 104158-11-4P, 3-Caren-4-yl sulfoxide(?)

RL: PREP (Preparation) (preparation of) 104158-11-4 CAPLUS

of

RN

CN 3-Caren-4-yl sulfoxide (7CI) (CA INDEX NAME)